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13. ABSTRACT *(Maximum 200 words)*

Three graduate students and one undergraduate student were supported to pursue research in the area of crystal growth and complement the research activities of AFOSR/DARPA MURI project on integrated intelligent modeling, design and control of crystal growth processes. One doctoral student worked on integrating the radiation heat transfer model into MASTRAPP, the crystal growth model developed by the Consortium for Crystal Growth Research. He also built a parallel processing algorithm. The other two Masters and one undergraduate students worked in the area of experimental methods to develop database for model validation. These students have developed a three-dimensional temperature field visualization technique using liquid crystals as tracers and digital imaging software for 3D reconstruction. Reconstruction of 3D field from a series of 2D images is a novel technique and can be used for flow and heat transfer analysis that is inherently three-dimensional and oscillatory, e.g., melt flow in Czochralski crystal growth.

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AASERT Grant No. F49620-95-1-0387

STUDENT AUGMENATION FOR CRYSTAL GROWTH RESEARCH

Principal Investigator:

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FINAL REPORT

STUDENT AUGMENATION FOR CRYSTAL GROWTH RESEARCH

Summary:

Three graduate students and one undergraduate student were supported to pursue research in the area of crystal growth and complement the research activities of AFOSR/DARPA MURI project on integrated intelligent modeling, design and control of crystal growth processes. One doctoral student worked on integrating the radiation heat transfer model into MASTRAPP, the crystal growth model developed by the Consortium for Crystal Growth Research. He also built a parallel processing algorithm. The other two Masters and one undergraduate students worked in the area of experimental methods to develop database for model validation. These students have developed a three-dimensional temperature field visualization technique using liquid crystals as tracers and digital imaging software for 3D reconstruction. Reconstruction of 3D field from a series of 2D images is a novel technique and can be used for flow and heat transfer analysis that is inherently three-dimensional and oscillatory, e.g., melt flow in Czochralski crystal growth.

OBJECTIVE

The primary objective of this AASERT program was to train two graduate students who are US citizens, in the area of crystal growth, complement the research activities of MURI award on "Integrated Intelligent Modeling, Design and Control of Crystal Growth Processes", and expand the activities of AFOSR/DARPA Consortium for Crystal Growth Research. In particular, one student was expected to work on parallelization of the crystal growth model being developed by the Consortium and the other student was expected to conduct validation experiments.

ACCOMPLISHMENTS

The AASERT grant has supported William Garber, a doctoral student in the Department of Applied Mathematics and Statistics, Paul Lutjen, and Robert White, MS students in mechanical engineering, and Matt Whiten, an undergraduate student in mechanical engineering. Garber is expected to complete his doctoral dissertation by the summer of 2000 and is continue to be supported through the MURI grant. Lutjen has already finished his Masters work and successfully presented his thesis in July 1999. White, on the other hand, left after one year of AASERT support and joined Yale University for doctoral studies. Whiten finished his BS in May 1998.

Garber's doctoral research concentrates on the parallelization of radiative heat transfer solver, and its integration with MASTRAPP2d, the code developed by the researchers of the Consortium for Crystal Growth. The results allowed him to independently refine the grids of the radiating interfaces in a crystal growth system. In the process of validation he discovered that the treatment of geometrical corners in the original serial code, his starting point for parallelization, was flawed, as the convergence under mesh refinement was very slow. He analyzed and fixed this problem by improving the integration routines near regions that are close and quite visible to each other.

Garber's research also involved improving the algorithms for tracking the moving interfaces and their intersections (notably the triple point where gas, melt and solid join). Triple point motion is one of the best observable in Czochralski growth, and is an important input to the control algorithm. For common materials, the growth direction has a constant angle to the meniscus at the triple-point. Therefore, an accurate determination of meniscus shape near the crystal is important. In the current version of MASTRAPP2d, the meniscus shape is assumed to be of a known shape and given by a function, an assumption that is limiting when the objective is to simulate diameter control of the crystal. In fact, the meniscus shape is determined by surface tension, rotation, triple point position, and angle to the wall (a less important quantity). Garber discovered that by parameterizing the meniscus as a function of angle (to a vertical) one has a well-posed equation for meniscus shape. He developed a robust, and provably convergent, algorithm for its solution. While the mathematical literature on meniscus problems is huge (related to minimal surfaces), the literature on numerical algorithms seems scant. He has compared his algorithm to a small number of other works available in the literature. The resulting parallel radiation code, using MPI as its parallel communication language has been validated and tested on a number of platforms: the IBM SP2 cluster in the Process Modeling

Laboratory, and the Galaxy super-computer in the Department of Applied Mathematics and Statistics at Stony Brook.

Paul Lutjen, on the other hand, worked on visualization and growth simulation experiments. The primary focus of this research is to develop an experimental technique to reconstruct three-dimensional field from two-dimensional images since only two-dimensional flow and temperature fields can be visualized, photographed and video-recorded using an optical method. Reconstruction of 3D field from a series of 2D images will be a novel technique and can be used for flow and heat transfer analysis that is inherently three-dimensional and oscillatory, such as crystal growth processes. Lutjen designed and built an experiment set-up in which the light sheet and video camera can be moved at given speeds either continuously or intermittently. Their movements are synchronized and independently controlled so that the adjustments can be made for the depth of field and the field of visualization can remain in focus. Lutjen has also performed a series of calibration experiments and obtained multiple slices for natural convection flows in a cubic enclosure. He selected an appropriate software that can perform the task of digitally reconstructing a three-dimensional field from two-dimensional images and developed an interface to transfer his experimental data to this software. Lutjen has been helped by an undergraduate student, Matt Whiten.

Stony Brook researchers have been able to develop a successful liquid crystal thermography technique to visualize the temperature field in a rotating system (simulating Czochralski growth) and process these images to obtain a broader spectrum of temperature bands, measure temperature oscillations and calculate thermal gradients. Lutjen built on this knowledge to make original contributions in this field.

Lutjen showed, for the first time, that liquid crystal thermography can be successfully used to conduct volumetric measurements of temperature fields. It has the ability to image even transient temperature field and produce temperature-time history. He was also able to calculate heat transfer rates using liquid crystal thermographs and digitized images that were never made possible. Non-invasive measurement of heat transfer coefficients is considered a major achievement.

PERSONNEL SUPPORTED

William Garber, a doctoral student in the Department of Applied Mathematics and Statistics, and Paul Lutjen and Robert White, MS students, and Matt White, an undergraduate student in the Department of Mechanical Engineering.

REFEREED PUBLICATIONS:

1. W. Garber and F. Tangerman, "Calculating Radiative Heat Transfer in an Axisymmetric Closed Chamber: An Application to Crystal Growth," Submitted to ***Journal of Crystal Growth*** (1999).

2. P. Lutjen, W., Clark, and V., Prasad, "Liquid Crystal Thermography and Scanning Flow Tomoscopy for Three-Dimensional Temperature Field Measurement," ***National Heat Transfer Conference,*** Albuquerque, 1999, also being submitted to ***Journal of Heat Transfer***.

3. D. Mishra, P. Lutjen, V. prasad, "A Tomographic Reconstruction Method for Three-Dimensional Liquid Crystal Thermography," ***International Mechanical Engineering Congress and Exhibits '99***, Albuquerque (1999), also being submitted to ***Journal of Heat Transfer***.

CONFERENCE PRESENTATIONS:

1. W. Garber, "Calculating Radiative Heat Transfer in an Axisymmetric Closed Chamber: An Application to Crystal Growth," New Trends in High Performance Computing, ***HPCU '99,*** August 1999, SUNY Stony Brook.

AUGMENTATION AWARDS FOR SCIENCE & ENGINEERING RESEARCH TRAINING (AASERT)
REPORTING FORM

The Department of Defense (DoD) requires certain information to evaluate the effectiveness of the AASERT Program. By accepting this Grant which bestows the AASERT funds, the Grantee agrees to provide 1) a brief (not to exceed one page) narrative technical report of the research training activities of the AASERT-funded student(s) and 2) the information should be provided to the Government's technical point of contract by each annual anniversary of the AASERT award date.

1. Grantee identification data: (R&T and Grant numbers found on Page 1 of Grant)

a. State University of New York at Stony Brook
University Name

b. F49620-95-1-0387
Grant Number

c. F49620-95-1-0387
R&T Number

d. Vishwanath Prasad
P.I. Name

e. From: 1 June 1995 To: 31 May 1999
AASERT Reporting Period

NOTE: Grant to which AASERT award is attached is referrred to hereafter as "Parent Agreement".

2. Total funding of the Parent Agreement and the number of full-time equivalent graduate students (FTEGS) supported bt the Parent Agreement during the 12-month period prior to the AASERT award date.

a. Funding: $ 84,768.00

b. Number FTEGS: None Supported from this Grant

3. Total funding of the Parent Agreement and the number of FTEGS supported by the Parent Agreement during the current 12-month period.

a. Funding: $ 1,000,000.00 (MURI Program)

b. Number FTEGS: 12 at Stony Brook

4. Total AASERT funding and the number of FTEGS and undergraduate students (UGS) supported by AASERT funds during the current 12-month reporting period.

a. Funding: $ 50,108.32

b. Number FTEGS: two

c. Number UGS: one

VERIFICATION STATEMENT: I hereby verify that all students supported by the AASERT award are U.S. Citizens.

Vishwanath Prasad
Principal Investigator

Date 8/30/99